

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 174 °C

Global applicability domain: Outside

Local applicability domain index: 5.66e-01

Confidence level: 5.86e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Diazabicyclo[2.2.2]octane

Measured: 174

Predicted: 174

Image not found

1,4-Dimethylpiperazine

Measured: 131

Predicted: 144

Image not found

1,3,4-Thiadiazole, 2,5-dimethyl-

Measured: 203

Predicted: 193

Image not found

Piperidine, 1-nitro-

Measured: 245

Predicted: 220